On the Unitary Representation of the Schrödinger Group Concerned with the Continuous Energy Spectrum*

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In relation to the quantum-mechanical eigenvalue problem in terms of a complete set of the Casimir operators the unitary representation of the Schrödinger group of the positive energy states of the hydrogen like atom will be given as an example of the continuous energy spectrum.

INFINITESIMAL OPERATORS OF THE SCHRODINGER GROUP

All of the integral operators commutative with non-relativistic Hamiltonian $H=\boldsymbol{p}^2/2m-Ze^2/r^2$ of the hydrogen like atom are, as is well-known, the Lenz-Pauli vector integral

$$\boldsymbol{A}=\frac{1}{2\beta}(\boldsymbol{M}\times\boldsymbol{p}-\boldsymbol{p}\times\boldsymbol{M})-\frac{\boldsymbol{r}}{r} \tag{1.1}$$

with usual notations and $\beta=Ze^2m$, in addition to the orbital angular momentum operator $\boldsymbol{M}=\boldsymbol{r}\times\boldsymbol{p}$, whose components are $M_\lambda=M_{\mu\nu}$ (λ, μ, and ν take respectively the whole values of 1, 2, and 3), where it is shown readily that the commutation relation between these six operators are given by

$$\begin{aligned}[A_\lambda,\ A_\mu] &= 2M_{\lambda\mu}m\beta^2H\\ [M_{\lambda\mu},\ A_\nu] &= \delta_{\mu\nu}A_\lambda-\delta_{\lambda\nu}A_\mu\\ [M_{\lambda\mu},\ M_{\mu\nu}] &= -i\hbar M_{\lambda\mu}.\end{aligned} \tag{1.2}$$

Now take the following infinitesimal operators:

$$\begin{aligned}F_{\lambda\mu}&=i\hbar^{-1}M_{\lambda\mu}\\ F_{4\lambda}&=-F_{\lambda4}=-i\hbar^{-1}(i/\beta p_0)A_\lambda\end{aligned} \tag{1.3}$$

as the generators of the Schrödinger group for the positive energy (continuous) states of the unbound electron, where $p_0=\sqrt{2mH'}$, H' being the eigenvalue of the Hamiltonian, then these operators satisfy the same commutation relations as satisfied by the infinitesimal operators of the four-dimensional Lorentz group,[1] viz. it is found that the Schrödinger group of the present case is isomorphic with the Lorentz group.

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Thereupon for convenience we substitute (1.3) for

$$\begin{aligned} F_\lambda &= -\hbar^{-1}M_{\mu\nu} \\ \tilde{F}_\lambda &= -i\hbar\, A_\lambda/\beta p_0, \end{aligned} \tag{1.4}$$

then it follows the commutation relations:

$$\begin{aligned} [F_\lambda,\ F_\mu] &= i\,F_\nu \\ [\tilde{F}_\lambda,\ \tilde{F}_\mu] &= -i\,F_\nu \\ [F_\lambda,\ \tilde{F}_\mu] &= -i\,\tilde{F}_\nu, \end{aligned} \tag{1.5}$$

while the remaining relations are all commutative. Hence it is our problem to find out the representation by the bases (1.4) of the Lie ring. It is shown that there must exist a set of two Casimir operators, since the present ring is the semi-simple one with the rank two.[2] In fact we have

$$\begin{aligned} G_1 &= \frac{1}{4}\sum_\lambda (F_\lambda{}^2 - \tilde{F}_\lambda{}^2) \\ G_2 &= \sum_\lambda F_\lambda \tilde{F}_\lambda. \end{aligned} \tag{1.6}$$

and it can be given that only G_1 has the following functional relation with the Hamiltonian:

$$G_1 = \frac{Z^2e^4m}{8\hbar^2H} + \frac{1}{4}, \tag{1.7}$$

while it can be derived from the metric fundamental tensor of the above ring that every eigenvalue of G_2 gives the value of zero. Therefore only representation connected with the eigenvalue of G_1 comes into our problem.

CONSTRUCTION OF THE REPRESENTATION MATRICES

The indefinite property of the present Casimir operator different from the case of the real rotation group brings about the result that the unitary representation with infinite degree of the Lorentz group[3] can be characterized by continuously variable parameters, while the well-known spinor representation is out of the question, because it is not unitary. And it should be noted that $\tilde{F}_\lambda$'s have continuous eigenvalues by the following consideration.

Now let us take

$$\mathrm{F}^+ = F_1 + i\,F_2, \quad \tilde{F}^+ = \tilde{F}_1 + i\,\tilde{F}_2, \tag{2.1}$$

then the commutation relations of

$$[\tilde{F}^+,\ \tilde{F}_3] = F^+, \quad [F^+,\ \tilde{F}_3] = -\tilde{F}^+ \tag{2.2}$$

can be found, and the representation diagonalizing $\tilde{F}_3$ is given by

$$
\begin{aligned}
(n''-n')(n'|\tilde{F}^{+}|n'') &= (n'|F^{+}|n''),\\
(n''-n')(n'|\tilde{F}^{+}|n'') &= -(n'|F^{+}|n'').
\end{aligned}
\tag{2.3}
$$

From both relations of (2.3) it follows

$$
(n''-n')^2=-1. \tag{2.4}
$$

This result means imaginary eigenvalues, but if n takes continuous values, such unreasonable result does not appear. Then the upper relation of (2.3) should be rewritten as follows:

$$
\begin{aligned}
&\int (n'|\tilde{F}^{+}|n''')\, n''dn'''\delta(n'''-n'')\\
&-\int n'\delta(n'-n''')\,dn'''(n'''|F^{+}|n'') = (n'|F^{+}|n'').
\end{aligned}
\tag{2.5}
$$

The similar relation comes into existence also for the lower relation of (2.3).

In order to find the explicit unitary representation we begin with the construction of the representation of the sub-ring including the elements of F_λ's only, and let us put

$$
F^{+}=F_1+i\,F_2,\quad F^{-}=F_1-i\,F_2, \tag{2.6}
$$

then the matrix elements of the irreducible representations are given by

$$
\begin{aligned}
(l,m|F^{+}|l',m') &= \sqrt{(l+m)(l-m+1)}\,\delta_{ll'}\,\delta_{m,m'+1}\\
(l,m|F^{-}|l',m') &= \sqrt{(l-m)(l+m+1)}\,\delta_{ll'}\,\delta_{m,m'-1}\\
(l,m|F_3|l',m') &= m\,\delta_{ll'}\,\delta_{mm'},
\end{aligned}
\tag{2.7}
$$

where the full representation space is nothing but the Hilbert space, then the above matrix elements should be reformed for the basic vectors $V_{g,l,m}$ ($l=0,1,2\ldots$ for every eigenvalue g of G_1), provided that we select the basic vectors in accordance with (2.7) to give the direct-sum space of the irreducible representations of the sub-ring with regard to F_λ:

$$
\begin{aligned}
(g,l,m|F^{+}|g',l',m') &= \sqrt{(l+m)(l-m+1)}\,\delta_{gg'}\,\delta_{ll'}\,\delta_{m,m'+1}\\
(g,l,m|F^{-}|g',l',m') &= \sqrt{(l-m)(l+m-1)}\,\delta_{gg'}\,\delta_{ll'}\,\delta_{m,m'-1}\\
(g,l,m|F_3|g',l',m') &= m\,\delta_{gg'}\,\delta_{ll'}\,\delta_{mm'}.
\end{aligned}
\tag{2.8}
$$

In the similar way the matrix elements of

$$
\tilde{F}^{+}=\tilde{F}_1+i\,\tilde{F}_2,\quad \tilde{F}^{-}=\tilde{F}_1-i\,\tilde{F}_2 \tag{2.9}
$$

is given by

$$
\begin{aligned}
(g,l,m|\tilde{F}^{+}|g',l',m') &= \{-a_l\sqrt{(l+m)(l-m+1)}\,\delta_{l,l'+1} \\
&+ b_l\sqrt{(l+m)(l-m+1)}\,\delta_{ll'} + a^*_{l+1}\sqrt{(l-m+1)(l-m+2)}\,\delta_{l,l'-1}\}\,\delta_{gg'}\,\delta_{m,m'+1} \\
(g,l,m|\tilde{F}^{-}|g',l',m') &= \{a_l\sqrt{(l-m)(l-m-1)}\,\delta_{l,l'-1} \\
&+ b_l\sqrt{(l+m)(l-m+1)}\,\delta_{ll'} - a^*_{l+1}\sqrt{(l+m+1)(l+m+2)}\,\delta_{l,l'+1}\}\,\delta_{gg'}\,\delta_{m,m'-1} \\
(g,l,m|\tilde{F}_3|g',l',m') &= \{a_l\sqrt{(l+m)(l-m)}\,\delta_{l,l'+1} \\
&+ b_l\cdot m\,\delta_{ll'} + a^*_{l+1}\sqrt{(l+m+1)(l-m+1)}\,\delta_{l,l'-1}\}\,\delta_{gg'}\,\delta_{mm'},
\end{aligned}
\tag{2.10}
$$

where a^*_l is the complex conjugate of a_l, while b_l is real. These coefficients can be determined by the use of the following commutation relation:

$$[\tilde{F}^{+},\ \tilde{F}^{-}] = -2\,F_3. \tag{2.11}$$

From the above relations (2.10) and (2.11)

$$
\begin{aligned}
(l-1)\,a_l b_{l-1} &= (l+1)\,a_l b_l \\
(l-1)\,a^*_l b_{l-1} &= (l+1)\,a^*_l b_l \\
(2l+3)\,a^*_{l+1}a_{l+1} - (2l-1)\,a^*_l a_l - b_l^2 &= 1
\end{aligned}
\tag{2.12}
$$

can be derived, and further from (2.8), (2.10), and (1.6) we find

$$
\begin{aligned}
&b_l = g'/\,l(l+1) \\
&(l+1)(2l+3)\,a^*_{l+1}a_{l+1} + l(2l-1)\,a^*_l a_l - l(l+1)(1-b_l^2) = 4g,
\end{aligned}
\tag{2.13}
$$

where g' is the eigenvalue of the Casimir operator G_2, but our problem is restricted by $g'=0$, then it follows

$$b_l = 0. \tag{2.14}$$

Consequently the coefficient a_l can be determined from

$$
\begin{aligned}
(2l+3)\,a^*_{l+1}a_{l+1} - (2l-1)\,a^*_l a_l &= 1 \\
(l+1)(2l+3)\,a^*_{l+1}a_{l+1} + l\,(2l-1)\,a^*_l a_l - l\,(l+1) &= 4g,
\end{aligned}
\tag{2.15}
$$

or

$$
\begin{aligned}
a^*_{l+1}a_{l+1} &= \frac{l(l+2)+4g}{(2l+1)(2l+3)} \\
a^*_l a_l &= \frac{(l-1)(l+1)+4g}{(2l-1)(2l+1)}.
\end{aligned}
\tag{2.16}
$$

However, these two formula are quite equivalent, and then $a^*_l = -\,a_l$ can be readily obtained:

$$a_l = i\sqrt{\frac{(l-1)(l+1)+Z^2e^4m/2\hbar^2H'+1}{(2l-1)(2l+1)}}$$
$$a^*_l = -i\sqrt{\frac{(l-1)(l+1)+Z^2e^4m/2\hbar^2H'+1}{(2l-1)(2l+1)}}. \qquad (2.17)$$

Thus the unitary representation in question could be settled completely.

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